

# Supplementary Information:

## Dynamics of topological phonon edge states in polymer chains and supramolecular lattices on surfaces

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### Supplementary Methods

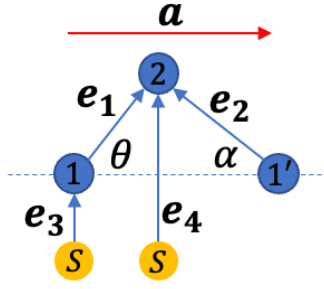
We used the dynamical matrix approach<sup>20</sup> to describe the linear response of our simplified mechanical systems. A  $d$ -dimensional frame consisting of  $N$  point masses connected by  $N_C$  springs is fully described by the compatibility matrix  $C$ , relating the  $Nd$ -dimensional vector of sites displacements  $\mathbf{u}$  to the  $N_C$ -dimensional vector of bond elongations  $\mathbf{e}$ :

$$C \cdot \mathbf{u} = \mathbf{e} \quad (1)$$

The normal modes of the system are the eigenvalues of the dynamical matrix  $\mathbf{D}$ , which is given by:

$$D = C^* \kappa C, \quad (2)$$

where  $\kappa$  is the  $N_C \times N_C$  diagonal matrix of spring constants.  $C^*$  denotes the conjugate transpose matrix of  $C$ . Bond elongations are obtained using,  $e_n = \hat{e}_n \cdot (\mathbf{u}_j - \mathbf{u}_i)$ , where  $\hat{e}_n$  is the unit vector pointing from site  $i$  to  $j$  in the undistorted lattice.



**Supplementary Schema 1:** aSSH model showing the elongation vectors  $e_n$  for the unit cell (dashed rectangle) characterized by the unit cell vector  $\mathbf{a}$  vector for the aSSH model. The substrates masses  $S$  are fixed.

For the aSSH case:

$$\mathbf{e}_1 = \hat{e}_1 \cdot (\mathbf{u}_1 - \mathbf{u}_2)$$

$$\mathbf{e}_2 = \hat{e}_2 \cdot (\mathbf{u}_2 - \mathbf{u}_1(\mathbf{r} + \mathbf{a}))$$

$$\mathbf{e}_3 = \hat{e}_3 \cdot \mathbf{u}_1$$

$$\mathbf{e}_4 = \hat{e}_4 \cdot \mathbf{u}_2$$

In this way we can construct the connectivity matrix:

$$\begin{pmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \end{pmatrix} = \begin{pmatrix} \hat{e}_{1x} & -\hat{e}_{1x} & \hat{e}_{1y} & -\hat{e}_{1y} \\ -e^{ik\cdot a}\hat{e}_{2x} & \hat{e}_{2x} & e^{ik\cdot a}\hat{e}_{2y} & -\hat{e}_{2y} \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} u_{1x} \\ u_{2x} \\ u_{1y} \\ u_{2y} \end{pmatrix} \quad (3)$$

where  $\mathbf{a}$  is the unit vector. In terms of the angles of Scheme 1 our connectivity matrix reads:

$$\mathbf{C} = \begin{pmatrix} \cos \theta & -\cos \theta & \sin \theta & -\sin \theta \\ -e^{ik\cdot a}\cos \alpha & \cos \alpha & e^{ik\cdot a}\sin \alpha & -\sin \alpha \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad (4)$$

Which allow us to construct, the dynamical matrix after equation 2:

D

$$= \begin{pmatrix} \cos \theta & -e^{-ik\cdot a}\cos \alpha & 0 & 0 \\ -\cos \theta & \cos \alpha & 0 & 0 \\ \sin \theta & e^{-ik\cdot a}\sin \alpha & 1 & 0 \\ -\sin \theta & -\sin \alpha & 0 & 1 \end{pmatrix} \begin{pmatrix} \kappa_1 & 0 & 0 & 0 \\ 0 & \kappa_2 & 0 & 0 \\ 0 & 0 & \kappa_3 & 0 \\ 0 & 0 & 0 & \kappa_4 \end{pmatrix} \begin{pmatrix} \cos \theta & -\cos \theta & \sin \theta & -\sin \theta \\ -e^{ik\cdot a}\cos \alpha & \cos \alpha & e^{ik\cdot a}\sin \alpha & -\sin \alpha \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$D_{aSSH} = \begin{pmatrix} D_{11} & D_{12} & D_{13} & D_{14} \\ D_{21} & D_{22} & D_{23} & D_{24} \\ D_{31} & D_{32} & D_{33} & D_{34} \\ D_{41} & D_{42} & D_{43} & D_{44} \end{pmatrix} \quad (5)$$

And the components:

$$\begin{aligned}
D_{11} &= D_{22} = \kappa_1 \cos^2 \theta + \kappa_2 \cos^2 \alpha \\
D_{12} &= -\kappa_1 \cos^2 \theta - \kappa_2 e^{-ik \cdot a} \cos^2 \alpha \\
D_{13} &= D_{24} = D_{31} = D_{42} = \kappa_1 \sin \theta \cos \theta - \kappa_2 \sin \alpha \cos \alpha \\
D_{14} &= D_{32} = -\kappa_1 \sin \theta \cos \theta + \kappa_2 e^{-ik \cdot a} \sin \alpha \cos \alpha \\
D_{21} &= -\kappa_1 \cos^2 \theta - \kappa_2 e^{ik \cdot a} \cos^2 \alpha \\
D_{23} &= D_{41} = -\kappa_1 \sin \theta \cos \theta + \kappa_2 e^{ik \cdot a} \sin \alpha \cos \alpha \\
D_{33} &= \kappa_1 \cos^2 \theta + \kappa_2 \cos^2 \alpha + \kappa_3 \\
D_{34} &= -\kappa_1 \sin^2 \theta - \kappa_2 e^{-ik \cdot a} \sin^2 \alpha \\
D_{43} &= -\kappa_1 \sin^2 \theta - \kappa_2 e^{ik \cdot a} \sin^2 \alpha \\
D_{44} &= \kappa_1 \cos^2 \theta + \kappa_2 \cos^2 \alpha + \kappa_4
\end{aligned}$$

Equation 5 can be can also written as a Hermitian matrix:

$$D_{aSSH} = \begin{pmatrix} D_{11} & D_{12} & D_{13} & D_{14} \\ D_{12}^* & D_{11} & D_{14}^* & D_{13} \\ D_{13} & D_{14} & D_{11} + \kappa_3 & D_{34} \\ D_{14}^* & D_{13} & D_{34}^* & D_{11} + \kappa_4 \end{pmatrix} \quad (6)$$

Similarly, for the daSSH model, the connectivity matrix is given by:

$$C = \begin{pmatrix} \cos \theta & -\cos \theta & \sin \theta & -\sin \theta & 0 & 0 \\ -e^{ik \cdot a} \cos \alpha & \cos \alpha & e^{ik \cdot a} \sin \alpha & -\sin \alpha & 0 & 0 \\ 1 - e^{ik \cdot a} & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 - e^{ik \cdot a} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \quad (7)$$

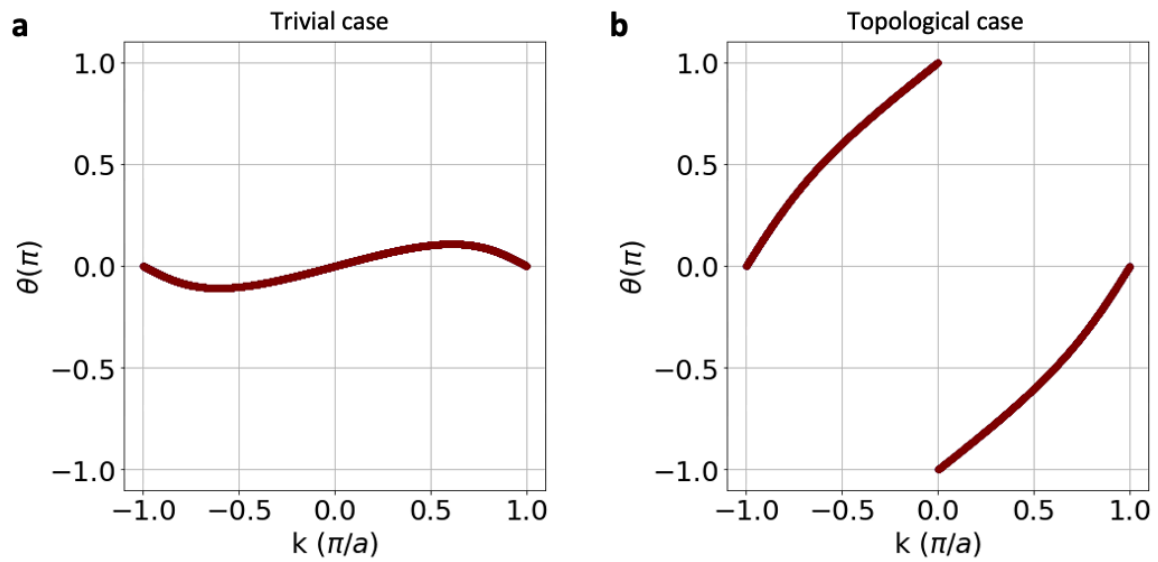
And the dynamical Hermitian matrix:

$$D_{daSSH} = \begin{pmatrix} D_{11} & D_{12} & D_{13} & D_{14} & 0 & 0 \\ D_{12}^* & D_{11} & D_{14}^* & D_{13} & 0 & 0 \\ D_{13} & D_{14} & D_{33} & D_{34} & 0 & 0 \\ D_{14}^* & D_{13} & D_{34}^* & D_{33} & 0 & 0 \\ 0 & 0 & 0 & 0 & \kappa_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & \kappa_6 \end{pmatrix} \quad (8)$$

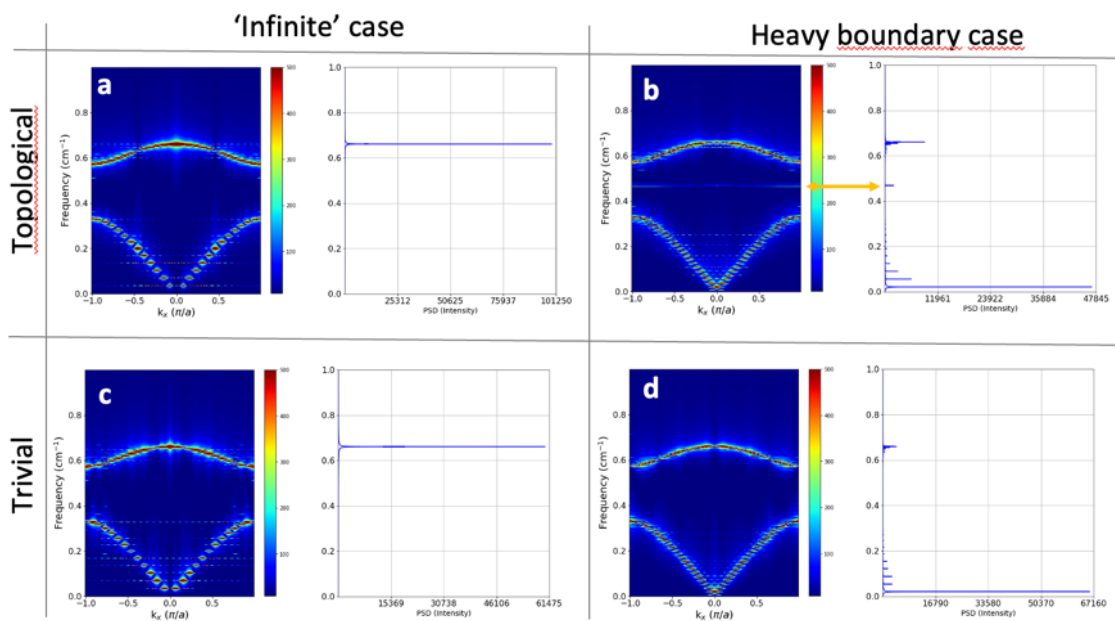
where the components are:

$$\begin{aligned}
D_{11} &= D_{22} = \kappa_1 \cos^2 \theta + \kappa_2 \cos^2 \alpha + \kappa_3 (1 - e^{-ik \cdot a})(1 - e^{ik \cdot a}) \\
D_{12} &= -\kappa_1 \cos^2 \theta - \kappa_2 e^{-ik \cdot a} \cos^2 \alpha \\
D_{13} &= \kappa_1 \sin \theta \cos \theta - \kappa_2 \sin \alpha \cos \alpha \\
D_{14} &= -\kappa_1 \sin \theta \cos \theta + \kappa_2 e^{-ik \cdot a} \sin \alpha \cos \alpha \\
D_{33} &= \kappa_1 \sin^2 \theta + \kappa_2 \sin^2 \alpha \\
D_{34} &= -\kappa_1 \sin^2 \theta - \kappa_2 e^{-ik \cdot a} \sin^2 \alpha
\end{aligned}$$

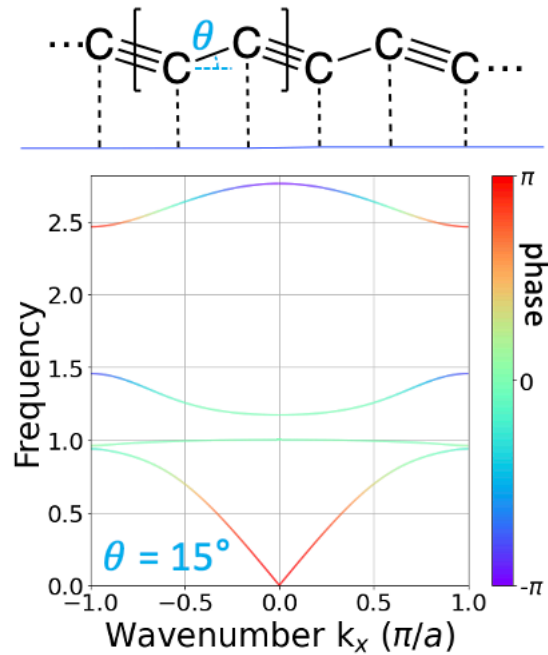
## Supplementary Figures



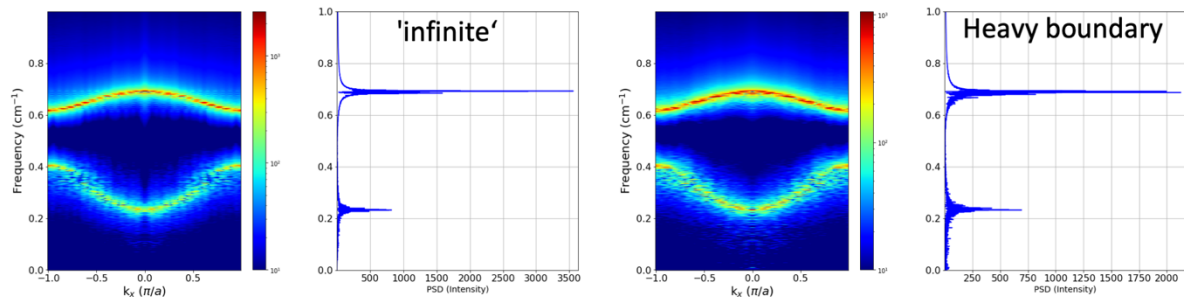
**Supplementary Figure 1.** Geometric phase for the trivial and topological pSSH model of Extended Data Fig. 1



**Supplementary Figure 2.** 1D phonon Su-Schrieffer-Heeger (pSSH) model, consisting on 52 mass chain of alternating spring constants  $\kappa_1$  and  $\kappa_2$ . For the topological (trivial) case  $\kappa_1 = 3000\text{kJ/mol}\cdot\text{nm}$  ( $1000\text{kJ/mol}\cdot\text{nm}$ ) and  $\kappa_2 = 1000\text{kJ/mol}\cdot\text{nm}$  ( $3000\text{kJ/mol}\cdot\text{nm}$ ). For the heavy boundary case the first and last mass are equal to  $100\text{au}$  and the rest are  $1\text{au}$ . For the infinite case all the masses are equal to  $1\text{au}$ .

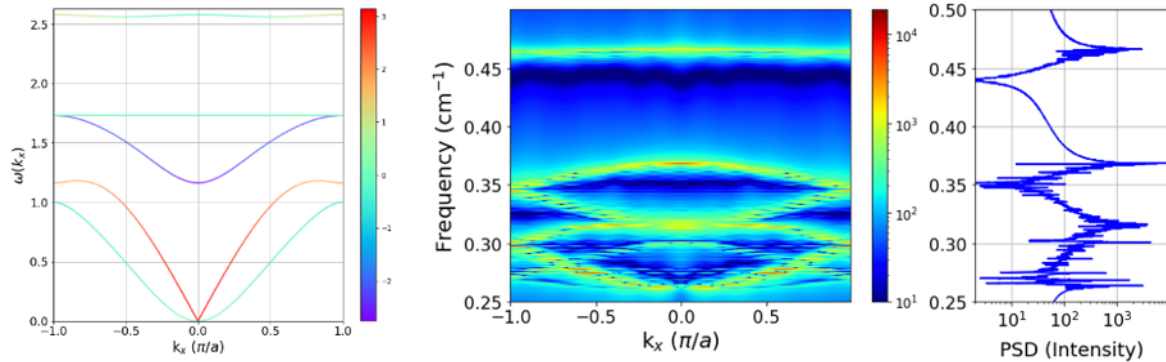


**Supplementary Figure 3.** aSSH model at equilibrium for a finite angle  $\theta=15^\circ$  between the masses and the substrate.

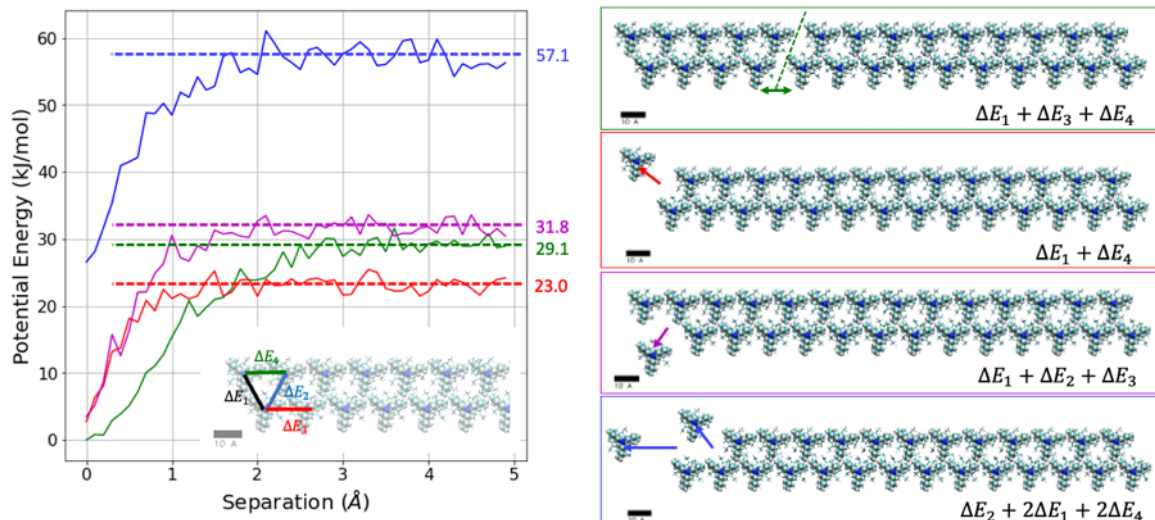


**Supplementary Figure 4.** Trivial case of aSSH model (Figure 2 of main text). The system consists of 52 mass chain of alternating spring constants  $\kappa_1$  and  $\kappa_2$ . For the topological (trivial) case  $\kappa_1 = 3000\text{kJ/mol}\cdot\text{nm}$  ( $1000\text{kJ/mol}\cdot\text{nm}$ ) and  $\kappa_2 = 1000\text{kJ/mol}\cdot\text{nm}$  ( $3000\text{kJ/mol}\cdot\text{nm}$ ), while

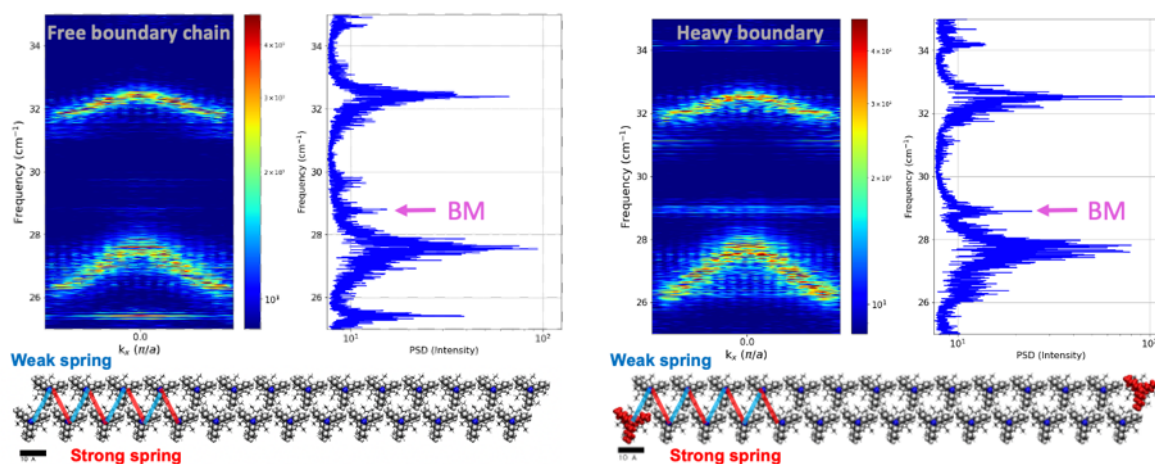
$\kappa_3 = 1000\text{kJ/mol}\cdot\text{nm}$  for all masses. For the heavy boundary case, the first and last masses are equal to 100au and the rest are 1au. For the infinite case, all the masses are equal to 1au. The substrate is harmonically restricted in 3D by a  $\kappa_{3D} = 10^6\text{ kJ/mol}\cdot\text{nm}$  in all three dimensions. The masses are restricted to move in a plane with a harmonic restriction of  $\kappa_y = 10^6\text{ kJ/mol}\cdot\text{nm}$ .



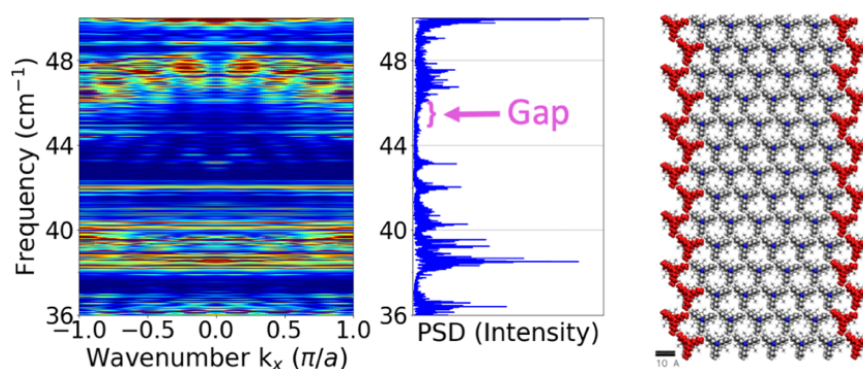
**Supplementary Figure 5.** Trivial case of daSSH model (Figure 4 of main text). The dynamical band structure on the left is generated using the parameters  $\kappa_1 = 1$ ,  $\kappa_2 = 3$ ,  $\kappa_3 = 3$  and  $\kappa_4 = \kappa_5 = 0.5$ ,  $\theta = \alpha = 60^\circ$  and  $m_c = 1$ . The MD band structure of the heavy boundary case for a system of 52 masses is showed on the right. Bond parameters:  $\kappa_1 = 1000\text{kJ/mol}\cdot\text{nm}$  (3000kJ/mol·nm in Figure 4) and  $\kappa_2 = 3000\text{kJ/mol}\cdot\text{nm}$  (1000kJ/mol·nm in Figure 4),  $\kappa_3 = 3000\text{kJ/mol}\cdot\text{nm}$ , and  $\kappa_5 = \kappa_6 = 500\text{kJ/mol}\cdot\text{nm}$ . The first and last masses are equal to 100au and the rest are 1au.



**Supplementary Figure 6.** Equivalent-spring constants from the realization of the daSSH model. From the dissociation energy plot, the interaction energies were calculated and equivalent springs constants determined.  $\Delta E_1 = 14.73$  kJ/mol,  $\Delta E_2 = 10.99$  kJ/mol,  $\Delta E_3 = 6.04$  kJ/mol,  $\Delta E_4 = 8.33$  kJ/mol. The atomistic top view in the inset starts with strong spring. The CHARMM potential energy was calculated every  $0.1\text{\AA}$  following the minimization algorithm L-BFGS.



**Supplementary Figure 7.** Trivial case for the Figure 4 of the main text. In both cases, the molecular chain starts with a weak spring. We identified a boundary mode in both free boundary and heavy boundary.



**Supplementary Figure 8.** Trivial case for the Figure 5 of the main text. Here the heavy boundary is next to a weak spring in alternating rows of the ribbon. We identified a gap in the region of interest.